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SPECTRAL METHODS FOR COMPRESSIBLE FLOW PROBLEMS

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SPECTRAL METHODS FOR COMPRESSIBLE FLOW PROBLEMS

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Abstract

In this article we review recent results concerning numerical simulation of shock waves using spectral methods. We discuss shock fitting techniques as well as shock capturing techniques with finite difference artificial viscosity. We also discuss the notion of the information contained in the numerical results obtained by spectral methods and show how this information can be recovered.

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Introduction

In the last decade spectral methods have been used very successfully in the numerical simulations of incompressible flows. Spectral methods have also emerged as a major tool in computational meteorology. This has led many researchers to look into the possiblity of applying spectral methods to simulate compressible flows that are of interest to aeronautical engineers. The aim of this article is to give a brief review of the major developments in this field in the last few years. In particular we would like to discuss the notion of the information that is contained in the numerical result. We argue that spectral methods yield more information about the exact solution than low order methods. This information is hidden in the form of numerical oscillations when the exact solution is discontinuous or contains extreme gradients. The structure of these wiggles depends on the nature of the discontinuity and, in some cases, a very accurate solution can therefore be extracted.

2. Spectral Methods

There are basically two steps in obtaining a numerical approximation $u_N(x)$ to a solution $u(x)$ of a differential equation. First, an appropriate finite or discrete respresentation of the solution must be chosen. This may take the form of an interpolating function between the values $u(x_j)$ at some suitable points x_j or a series coefficient in the finite representation

$$u_N(x) = \sum_{k=0}^{N} a_k \, \phi_k(x) \tag{2.1}$$

with given expansion functions $\phi_k(x)$. The second step is to obtain equations for the discrete values $u_N(x_j)$ or the coefficients a_k from the original equations. This second step involves finding an approximation for the differential operator in terms of the grid point values of u_N or, equivalently, the expansion coefficients. For example, the pseudospectral Chebyshev approximation to the equation

$$\begin{aligned} &u_t = u_x, && |x| < 1 \\ &u(x,0) = u_0(x), && u(1,t) = h(t) \end{aligned} \tag{2.2}$$

is obtained in the following manner. For a given time t we assume that $\{u_N(x_j,t)\}$ is known where $x_j = \cos\frac{\pi j}{N}$. We then interpolate these values to get

$$u_N(x,t) = \sum_{j=0}^{N} u_N(x_j,t)\ g_j(x) \tag{2.3}$$

where

$$g_j(x) = \frac{(-1)^{j+1}}{N^2}\frac{(1-x^2)T_N'(x)}{c_j(x-x_j)}, \qquad \begin{aligned} &c_0 = c_N = 2 \\ &c_j = 1, \qquad 0 < j < N. \end{aligned}$$

Note that $g_j(x_k) = \delta_{jk}$. Equivalently, since

$$g_j(x) = \frac{2}{N}\sum_{n=0}^{N}\frac{T_n(x_j)\ T_n(x)}{c_n}$$

where $T_n(x) = \cos(n \cos^{-1} x)$ is the Chebyshev polynomial of degree n, one

gets

$$u_N(x,t) = \sum_{n=0}^{N} a_n T_n(x)$$
$$a_n = \frac{2}{c_n N} \sum_{j=0}^{N} u(x_j,t) \frac{\cos(\pi jn/N)}{c_j}, \qquad j = 0,\cdots,N. \tag{2.4}$$

The next step is to differentiate (2.3) to get the system of ordinary differential equations

$$\frac{\partial u_N(x_k,t)}{\partial t} = \sum_{j=0}^{N} u_N(x_j,t) g_j'(x_k), \qquad j = 1,\cdots,N$$
$$\frac{\partial u_N}{\partial t}(x_0,t) = h'(t) \tag{2.5}$$

or using (2.4)

$$\frac{\partial u_N(x_k,t)}{\partial t} = \sum_{n=0}^{N} a_n T_n'(x_k) = \sum_{n=0}^{N-1} b_n T_n(x_k), \quad j = 1,\cdots,N$$
$$\frac{\partial u_N}{\partial t}(x_0,t) = h'(t) \tag{2.6}$$

where

$$b_N = 0, \qquad b_{N-1} = 2N\, a_N, \qquad b_n = \frac{1}{c_n} b_{n+2} + 2(n+1)a_{n+1} \cdot$$

Equations (2.5) and (2.6) are, in fact, identical. Equation (2.5) points out the possibility of applying the pseudospectral Chebyshev method by mulitplying the vector $u(x_j,t)$ by the matrix $g_j'(x_n)$ whereas the asymptotically efficient implementation of (2.6) is by using a Fast Fourier Transform.

In general, consider the system of equations

$$u_t = L(u)$$
$$u(t=0) = u_0, \tag{2.7}$$

where L is a nonlinear operator that involves only spatial derivatives. In spectral methods we define a finite dimensional subspace B_N which is the space of polynomials (or trigonometric polynomials) of degree N, and a projection operator P_N that maps the original space to B_N. An example of such a P_N is given in (2.3). In fact, given a function $f(x)$, $-1 < x < 1$, then (2.3) defines $P_N f = \sum_{j=0}^{N} f(x_j)g_j(x)$.

We then seek a solution u_N belonging to B_N such that

$$\frac{\partial u_N}{\partial t} = P_N L(u_N),$$
$$u_N(t=0) = P_N u_0. \tag{2.8}$$

For a more complete description of spectral methods we refer the reader to [3], [6].

Spectral methods are global in nature, i.e., in order to get an expression for $\frac{\partial}{\partial x} u_N$ we use all the grid points x_k, $k = 0,\cdots,N$ (see (2.5)). Together with the choice of the points x_k this explains their high order accuracy. The accuracy of spectral methods depends on the total number of points N, and the number of smooth derivatives of u. For smooth flows, great savings of

computer storage and time is gained by using spectral methods since only a small number of grid points is required to get the same accuracy obtained by other methods.

3. Spectral Methods and Shock Waves

The use of any formal high order method for the numerical simulation of flows with shocks poses theoretical and practical problems. The error estimates obtained for spectral methods depend on the smoothness of the solution and it is not clear at all that any degree of accuracy can be achieved for discontinuous solutions. On the one hand, it has been proven that for linear problems, high accuracy can be maintained within spectral methods far away from the discontinuity; on the other hand, it may be thought that for nonlinear problems the overall accuracy in the presence of discontinuities is limited to first order. However, in [10] Lax has argued that more information about the solution is contained in high resolution schemes, even in the nonlinear case. In fact, Lax has shown that the ε-capacity of the set of approximate solutions is closer to the ε-capacity of the set that includes the projections of exact solutions if the numerical scheme is a high order scheme. Typically, when a spectral method is used to simulate flows with shocks it yields an oscillatory solution. The oscillations are global, that is they occur not only in the neighborhood of the shock but all over the flow field. Several methods of overcoming these oscillations were suggested. Historically, the first attempts to get nonoscillatory results concentrated on using finite difference type artificial

dissipation. Taylor, et al. [15] used the method of Boris and Book of adding diffusion and antidiffusion terms for some model problems. Sakell [12] has checked a version of the Von Neumann-Richtmyer artificial dissipation for the wedge flow problem. Cornille [2] has used a version of the Lax-Wendroff scheme with inherent dissipation. Zang and Hussaini [16] simulated slightly viscous flows and treated the viscosity term by finite differences. Two real life flows were simulated using the above ideas. Reddy [11] introduced Fourier representation in the azimuthal direction in the three-dimensional Navier-Stokes code of Pulliam and Steger. In this problem there is enough dissipation coming from the discretization in the other directions. Reddy reports substantial improvement over the finite difference code. Streett [14] simulated transonic flow around an airfoil. His code is a full potential algorithm with retarded density. His results indicate that for subsonic flows, spectral methods are superior to the finite difference codes, whereas for transonic flow they are comparable. The results obtained by these methods indicate that a highly structured flow field is well-represented along with the front of the shock. However, the shock profiles are smeared and the accuracy in the smooth part of the flow is perhaps no longer spectral.

A different approach advocated first by Hussaini, Salas and Zang [9] is to fit the shock. This approach has been used to simulate various physical problems, most of them concerned with shock wave interactions. Since they were interested in the behavior of the flow on only one side of the shock, a coordinate transformation was employed so that the shock wave became a coordinate boundary. The Rankine-Hugoniot conditions were used both to determine the flow variables immediately upstream of the shock and to

determine the shock position. Since all the physical quantities on the downstream of the shock were prescribed the flow variables on the upstream side were obtained from the Rankine-Hugoniot relations. Note that the shock boundary is supersonic and therefore all the quantities must be specified and no special boundary treatment is necessary. The fluid motion was modeled by the two-dimensional Euler equation in nonconservation form. Also a spectral filtering in which the high modes were filtered every fifty time steps was employed to avoid nonlinear instability. Beautiful results were obtained for various shock interactions and for the blunt body problem.

In the third approach proposed in a forthcoming paper by Abarbanel and Gottlieb, the oscillations are being used to recover accurate information about the solution. Oscillations may arise from different sources; e.g., incorrect treatment of the boundaries in hyperbolic systems; nonlinear instabilities, etc. Usually these oscillations build up and finally cause explosive instabilities. One interesting class of numerical oscillations occur when flows with extreme gradients or local discontinuities are simulated. This type of oscillations does not cause instabilities even after many time steps. It has been observed (see [7]) that the wiggles are caused by the fact that the mesh is not fine enough to resolve the sharp gradients. In the case of a finite gradient a local refinement of the mesh often gets rid of the wiggles. For a very impressive demonstration of this fact, see [17]. Of course for a shock wave, no refinement of the mesh can remove the oscillations.

To better understand the origin of the oscillatory solution, consider the model equation

$$u_t = u_x$$
$$u(x,0) = H(x,x_\ell) \tag{3.1}$$

where $H(x,x_\ell)$ is the Heaviside function

$$H(x,x_\ell) = 0 \qquad x < x_\ell$$

$$H(x,x_\ell) = 1 \qquad x > x_\ell$$

$$X_\ell = \cos \frac{\pi}{N} (\ell + 1/2), \qquad \ell \text{ integer.}$$

When (3.1) is discretized by the pseudospectral Chebyshev method we get as the initial condition

$$u_N(x,0) = S(x,x_\ell) = \sum_{k=0}^{N} A_k T_k(x) \tag{3.1a}$$

where $T_k(x)$ is the Chebyshev polynomial of order k, and

$$A_0 = \frac{1}{N} (\ell + 1/2), \qquad A_N = \frac{1}{2N} \sin \pi(\ell + 1/2)$$

$$A_k = \frac{1}{N} \sin \frac{k\pi}{N} (\ell + 1/2)/\sin \frac{k\pi}{2N}, \qquad 1 < k < N-1.$$

At the grid points, $x_j = \cos \frac{\pi j}{N}$

$$S(x_j,x_\ell) = H(x_j,x_\ell),$$

Thus, no oscillations occur. However, after the numerical solution is convected by equation (3.1), it becomes oscillatory. This is because initially it is oscillatory between the grid points (see Fig. 1). Observe that the oscillations disappear when the discontinuity is exactly in the middle between two grid points. This demonstrates the fact that the structure of the oscillations provides information about the position and magnitude of the shock.

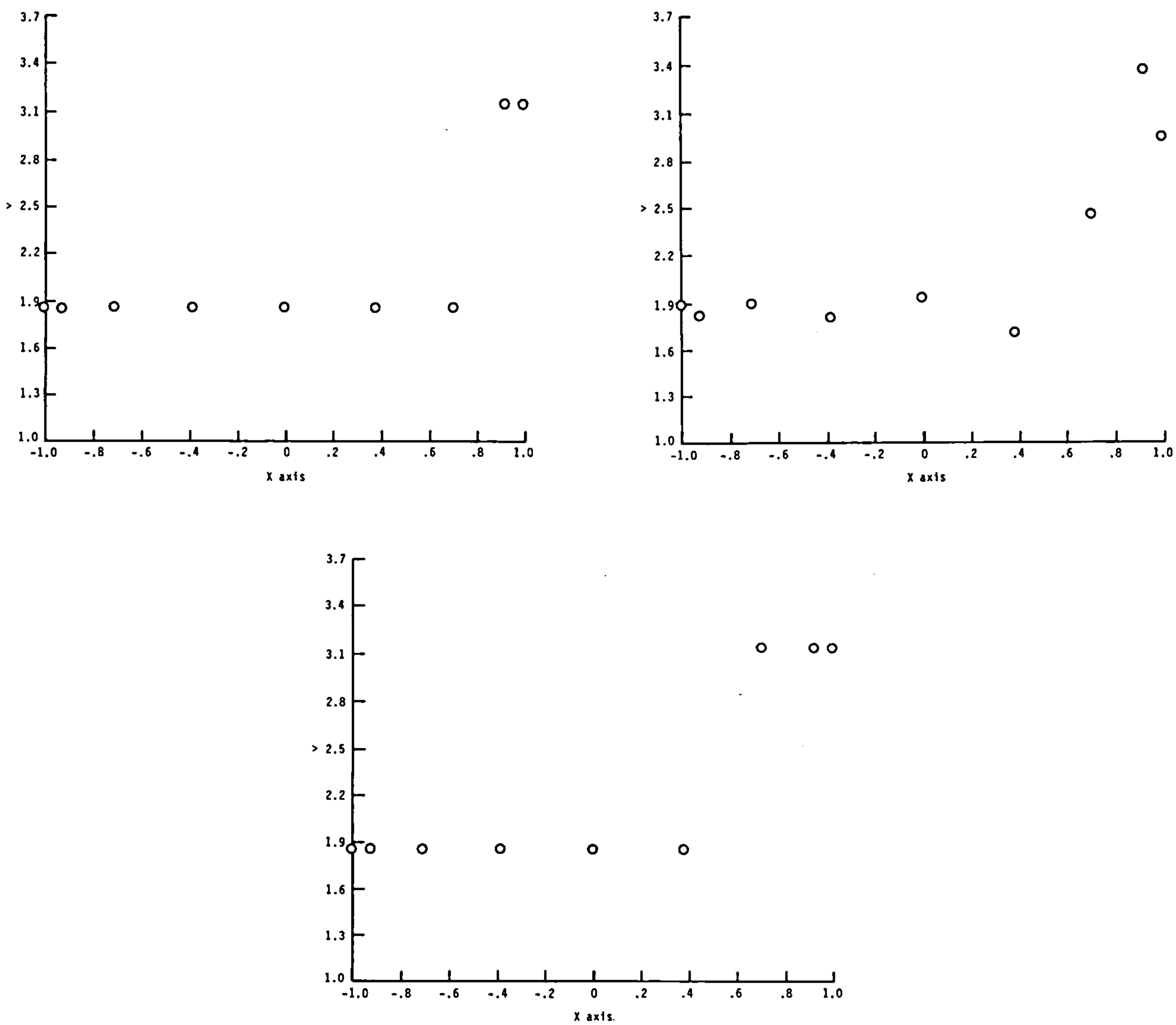

Figure 1

In general, consider (2.7) - (2.8) where now L is a linear operator and u_0 is discontinuous. From the last example it is clear that u_N does not approximate well $P_N u$ since $P_N u$ coincides with u at the grid points. We introduce an auxiliary equation

$$\frac{\partial v}{\partial t} = Lv$$
$$v(t=0) = P_N u_0. \tag{3.2}$$

For fixed N, v is a smooth function in contrast to the solution u of (2.7). We argue that u_N approximates (at the grid points) v rather than u. In fact from (2.8) and (3.2) one gets

$$\frac{\partial}{\partial t}\left(u_N - P_N v\right) = P_N LP_N\left(u_N - P_N v\right) + P_N L\left(P_N v - v\right)$$
$$(u_N - P_N v)(t=0) = 0. \tag{3.3}$$

Thus

$$u_N - P_N v = \int_0^t \left[\exp P_N LP_N(t - \tau)\right]\left[P_N L\left(P_N v(\tau) - v(\tau)\right)\right]d\tau.$$

The operator $\exp P_N LP_N(t - \tau)$ is bounded. This is, in essence, the notion of stability. The term

$$P_N L\left(P_N v - v\right)$$

is small because v is a smooth function. This shows that u_N approximates P_N v, hence at the grid points u_N approximates v.

In the last example we have demonstrated the fact the v is, in general, oscillatory. It is therefore no surprise that u_N is oscillatory. It is also clear that the structure of the oscillations may be used to extract a better approximation to u.

We will demonstrate now the possibility of extracting information from an oscillatory solution even in the nonlinear case. The physical problem is the well-known wedge flow. A plate is inserted in a uniform flow, and an oblique shock develops. The time dependent Euler equations in two-space dimensions were discretized by the pseudospectral Chebyshev method in space with a 9×9 grid and a modified Euler scheme was used for the time discretization (see [5]). Since we are interested in the steady state only, the accuracy of the time integration is of no importance. In order to be sure that a steady state is reached the code was run until all the physical quantities did not change to 11 significant figures over a span of 100 time steps. The values of the density in the steady state at the grid points together with the grid points themselves are given in Fig. 2.

	ρ									Y
	1.862	1.851	1.869	1.871	1.837	1.865	1.892	1.885	1.878	1.
	1.862	1.870	1.867	1.820	1.870	1.954	1.899	1.803	1.759	.961
	1.862	1.854	1.852	1.904	1.877	1.770	1.782	1.864	1.900	.853
	1.862	1.871	1.876	1.812	1.838	1.969	1.975	1.884	1.841	.691
	1.862	1.848	1.842	1.935	1.899	1.703	1.710	1.890	1.984	.5
	1.862	1.883	1.894	1.729	1.832	2.429	2.994	3.255	3.316	.308
	1.862	1.808	1.810	2.387	3.133	3.375	3.224	3.054	3.002	.146
	1.862	2.115	2.868	3.288	3.176	2.965	3.006	3.136	3.187	.038
	1.862	3.083	3.046	2.975	3.087	3.108	3.024	3.013	3.016	0
X	0	.038	.146	.308	.5	.691	.853	.961	1.	

Figure 2

Note that at the stations: $x_0 = 1$; $x_1 = .9619$; $x_2 = .85355$, the jump takes place between the grid points $y = .3086$ and $y = .5$, whereas the corresponding correct shock location is $y = .434$ for x_0, $y = .417$ for x_1 and $y = .370$ for x_2. Note also that the oscillatory behavior of the density is very similar to the behavior of $P_N\, v$, the solution of (3.2) at the grid points (see Fig. 1).

We therefore fit a step-function of the form $d_1 + d_2\, S(y,y_\ell)$ where $S(y,y_\ell)$ is defined in (3.1a) to the numerical results $\rho(y)$ in Fig. 2, at any station x_j, regarding d_1, d_2 and ℓ as unknowns. This yields three equations

$$\begin{aligned} d_1\, f_0 + d_2\, f_1 &= S_1 \\ d_1\, f_1 + d_2\, f_2 &= S_2 \\ d_1\, f_4 + d_2\, f_3 &= S_3 \end{aligned} \tag{3.4}$$

where

$$f_0 = N;\quad f_1 = \sum_{j=0}^{N} S(y_j,y_\ell)\,\frac{1}{c_j}\,;\qquad f_2 = \sum_{j=0}^{N} S(y_j,y_\ell)^2\,\frac{1}{c_j}\,;$$

$$f_3 = \sum_{j=0}^{N} S(y_j,y_\ell)\,\frac{\partial}{\partial \ell}\,S(y_j,y_\ell)\,\frac{1}{c_j}\,;\qquad f_4 = \sum_{j=0}^{N} \frac{\partial S}{\partial \ell}\,(y_j,y_\ell)\,\frac{1}{c_j}\,;$$

$$S_1 = \sum_{j=0}^{N} \rho(y_j)\,\frac{1}{c_j}\,;\qquad S_2 = \sum_{j=0}^{N} \rho(y_j) S(y_j,y_\ell)\,\frac{1}{c_j}\,;$$

$$S_3 = \rho(y_j)\,\frac{\partial S}{\partial \ell}\,(y_j,y_\ell).$$

Equation (3.4) yields the following nonlinear equation for the shock location y_ℓ

$$\begin{vmatrix} f_0 & f_1 & S_1 \\ f_1 & f_2 & S_2 \\ f_4 & f_3 & S_3 \end{vmatrix} = 0 \qquad (3.5)$$

Surprisingly, from (3.5) we recover the correct location of the shock at each x-station within the fourth significant digit. In this sense the information is indeed hidden in the form of oscillations.

It should be noted that in (3.4) we do not use the point values of $\rho(y)$ but rather the quantities S_1, S_2, S_3 which are equivalent to the integral of $\rho(y)$ against 1, $S(y,y_\ell)$ and $\frac{\partial}{\partial \ell}\,S(y,y_\ell)$. If $\rho(y)$ approximates well the first N modes of the solution $\rho_{ext}(y)$, then

$$\int_{-1}^{1} \big(\rho(y) - \rho_{ext}(y)\big)\,\frac{\phi(y)}{\sqrt{1-y^2}} = 0$$

where $\phi(y)$ is either 1 or $S(y,y_\ell)$ or $\frac{\partial S}{\partial \ell}\,(y,y_\ell)$. This may be the reason for the highly accurate values of the location of the shock obtained by (3.4).

Finally, we would like to describe another way of recovering correct point values from an oscillatory approximation. For simplicity we consider the spectral Legendre method although this idea has been generalized to other

spectral methods. Our approach is motivated by the work of Mock and Lax (see [10]).

Suppose that $f(x)$ is a C^∞ function at $|x| < 1$ except for one point of discontinuity. Suppose also that $f(x)$ has the following expansion in terms of the Legendre polynomials

$$f(x) = \sum_{k=0}^{\infty} a_k P_k(x)$$

and that

$$f_N(x) = \sum_{k=0}^{N} a_k P_k(x).$$

Even for large N, $f_N(x)$ is an oscillatory function. Let y be a point such that $f(x)$ is C^∞ in the interval $y-\varepsilon < x < y+\varepsilon$. Let

$$\psi(x) = \begin{cases} \frac{1}{\varepsilon} (1 - \xi^2)^q \sum_{k=0}^{P} (2k+1)P_k(0)P_k(\xi) & |\xi| < 1 \qquad \xi = \frac{x-y}{\varepsilon} \\ 0 & |\xi| > 1 \end{cases} .$$

It is clear that

$$\int_{-1}^{1} f_N(x)\psi(x)dx = \int_{-1}^{1} f(x)\psi(x)dx + \int_{-1}^{1} (f_N - f)\psi dx.$$

The function $\psi(x)$ has the expansion

$$\psi(x) = \sum_{k=0}^{\infty} b_k P_k(x)$$

and since $\psi(x)$ has $q-1$ continuous derivative the function $\psi_N(x)$

$$\psi_N(x) = \sum_{k=0}^{N} b_k P_k(x)$$

approximates ψ with high accuracy. Moreover, since $\psi_N(x)$ is a polynomial of degree N

$$\int_{-1}^{1} (f_N - f)\psi dx = \int_{-1}^{1} (f_N - f)(\psi - \psi_N)dx < \| f - f_N \| \, \| \psi - \psi_N \|$$

$$< \kappa \frac{\| \psi^{(q-1)} \|}{N^{q-1}} .$$

The last estimate can be found in [1].

It is therefore clear that

$$\int f_N \psi \, dx = \int f\psi \, dx + E_1$$

where E_1 is small. Moreover,

$$\int_{-1}^{1} f(x)\psi(x)dx = \int_{-1}^{1} f(y+\varepsilon\xi)(1-\xi^2)^q \sum_{k=0}^{P} (2k+1)P_k(0)P_k(\xi)d\xi.$$

Let

$$g(\xi) = f(y + \varepsilon\xi)(1- \xi^2)^n .$$

$g(\xi)$ is a C^∞ function for $|\xi| < 1$ and therefore has a rapidly converging expansion of the form

$$g(\xi) = \sum_{k=0}^{\infty} c_k \, P_k(\xi).$$

Therefore

$$\int_{-1}^{1} g(\xi) \sum_{k=0}^{p} (2k+1)P_k(0)P_k(\xi)d\xi = \sum_{k=0}^{p} c_k \, P_k(0)$$

$$= g(0) - \sum_{k=p+1}^{\infty} c_k = f(y) + E_2.$$

This shows that

$$\int f_N \, \psi \, dx$$

approximates $f(y)$ to a high order of accuracy. This filter had been successfully used by Gottlieb and Gruberger for several problems.

In conclusion we have demonstrated that numerical solutions obtained by spectral methods contain information about the correct solution that may be extracted to yield a high order approximation in the regular sense.

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16. Abstract

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